REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
18-07-2010	Final Report	1-Sep-2006 - 30-Jun-2010

4. TITLE AND SUBTITLE
Solvers and Calibration Methods for Ground and Surface Water Models

5a. CONTRACT NUMBER W911NF-06-1-0412

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER 611102

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S) ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S) 49381-MA.4

12. DISTRIBUTION AVAILABILITY STATEMENT
Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
The activities of this project are focused on (1) solving the nonsmooth nonlinear least squares problems that arise in the calibration of groundwater and surface water models, (2) nonlinear solvers for non-Darcy models of saturated groundwater flow, (3) continuation of previous work on solvers and preconditioners for unsaturated flow simulations. In the course of the project the PI and his students have completed work on non-Darcy flow models, graduating one student in the process, integrated proper orthogonal decomposition (POD) reduced order models

15. SUBJECT TERMS
Nonlinear equations, unsaturated flow, subsurface flow, multiphase flow, temporal integration, optimization

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
UU	UU	UU	UU		Carl Kelley
					19b. TELEPHONE NUMBER 919-515-7163

Report Title

Solvers and Calibration Methods for Ground and Surface Water Models

ABSTRACT

The activities of this project are focused on (1) solving the nonsmooth nonlinear least squares problems that arise in the calibration of groundwater and surface water models, (2) nonlinear solvers for non-Darcy models of saturated groundwater flow, (3) continuation of previous work on solvers and preconditioners for unsaturated flow simulations. In the course of the project the PI and his students have completed work on non-Darcy flow models, graduating one student in the process, integrated proper orthogonal decomposition (POD) reduced order models into optimization problems for saturated flow using the ERDC three-dimensional ADH code, and published a large comparative study of optimization methods as applied to a suite of problems in subsurface flow and transport. One student has been hired by the US Army Corps of Engineers and is now completing his thesis while on the staff at ERDC.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

M. Gee, C. T. Kelley, and R. B. Lehoucq, Pseudo-Transient Continuation for Nonlinear Transient Elasticity
International Journal for Numerical Methods in Engineering, 78, 2009, 1209-1219.

X-L Luo, C. T. Kelley, L-Z. Liao, and H-W Tam,
Combining Trust Region Techniques and Rosenbrock Methods for Gradient Systems
JOTA, 140, 2009, 265--286.

L-H. Zhang, C. T. Kelley, and L.-Z. Liao, 2007, A continuous Newton-type method for unconstrained optimization
Pacific J. Opt., 4, 2008, 259-277.

K. R. Fowler, J. P. Reese, C. E. Kees, J. E. Dennis, C. T. Kelley, C. T. Miller, C. Audet, A. J. Booker,
G. Couture, R. W. Darwin, M. W. Farthing, D. E. Finkel, J. M. Gablonsky, G. Gray, and T. G. Kolda
A Comparison of Derivative-Free Optimization Methods for Groundwater Supply and Hydraulic Capture Problems,
Advances in Water Resources, 31, 2008, 743-757.

C. T. Kelley, L-Z. Liao, L. Qi, M. T. Chu, J. P. Reese, and C. Winton, Projected Pseudo-Transient Continuation,
SIAM J. Numer. Anal., 46, 2008, 3071-3083.

Number of Papers published in peer-reviewed journals: 5.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

Number of Papers published in non peer-reviewed journals: 2.00

(c) Presentations

Pseudo-Transient Continuation (Kelley)

* SIAM Annual Meeting, San Diego, July 2008
* Copper Mt Conference on Iterative Methods, April 2008
* Third International Conference of Applied Mathematics, Plovdiv, Bulgaria, August 2007
* SIAM 2007 Conference on Computational Science and Engineering, Feb 2007

Implicit Filtering (Kelley)

* ISMP, Chicago, IL, August 2009
* AIM Workshop on Derivative-Free Hybrid Optimization Methods for Solving Simulation-Based Problems in Hydrology, October 2008.
* SIAM Conference on Optimization, May 2008

Model Calibration and POD (Kelley)

* Sixth East Asia SIAM Conference, Kuala Lumpur, Malaysia, June 2010
* Workshop for the 60th birthday of Prof. E. W. Sachs, Trier, Germany, June 2010
* IFIP Working Group 2.5 Symposium, Raleigh, NC, September 2009
* SIAM Conference on the Geosciences, June 2009
* International Conference on Engineering and Computational Mathematics, Hong Kong, China, May 2009.
* Oberwolfach Conference on Numerical Methods for Optimization Problems with PDE Constraints, January 2009
* SIAM Conference on the Geosciences, March 19, 2007

POD Calibration for ADH (Winton)
* Copper Mt Conference on Iterative Methods, April 2008
* SIAM Conference on Optimization, May 2008
* CMWR Conference, San Francisco, July 2008

Number of Presentations: 17.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

C. T. Kelley, C. Winton, O. J. Eslinger, and J. Pettway}, Calibration of ground water models with POD, in Numerical Techniques for Optimization Problems with PDE constraints, M. Heinkenschloss, R. H. W. Hoppe, and V. Schultz, eds., 2009, pp. 47--49.

Rank-Deficient and Ill-Conditioned Nonlinear Least Squares Problems, C. T. Kelley, I. C. F. Ipsen, and S. R. Pope, Proceedings of 2010 East Asian Section of SIAM, to appear.

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts): 2

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

(d) Manuscripts

Nonlinear Least Squares Problems and Subset Selection, I. C. F Ipsen, C. T. Kelley, and S. R. Pope, submitted for publication, 2010

Number of Manuscripts: 1.00

Patents Submitted

Patents Awarded

Graduate Students

NAME	PERCENT_SUPPORTED
Anna Meade	0.10
Corey Winton	0.80
Jill Reese	0.05
FTE Equivalent:	**0.95**
Total Number:	**3**

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Carl Kelley	0.05	No
FTE Equivalent:	**0.05**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:......	0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:......	0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):......	0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:......	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:......	0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME	
Corey Winton (expected 2010)	
Total Number:	**1**

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Final Progress Report for Army Research Office grant
W911NF-06-1-0412
Solvers and Calibration Methods for Ground and Surface Water Models
Reporting period: 09/01/06 – 07/31/10

Contents

1 Problems Studied

The objective of the project is to extend the PI's work on nonsmooth nonlinear equations from applications to solvers and temporal integration to into nonsmooth nonlinear least squares problems. The motivating application is calibration of models for both groundwater and surface water flow. A secondary objective is for the PI to continue his work on solvers and preconditioners for unsaturated flow and non-Darcy models of saturated flow.

The research is part of a collaboration with a group at the Coastal and Hydraulics Laboratory (CHL) at the US Army Engineer Research and Development Center (ERDC) on Adaptive Hydrology model (ADH), a production groundwater modeling code, will be used as both a large-scale testbed for the algorithmic work in the project and as a source for new research topics. The work done by the PI and his students has had a direct impact on the evolution of ADH and we expect that the proposed program of basic research will have an impact on the future of the code. Our collaborators at ERDC include Charlie Berger, Owen Eslinger, Matthew Farthing, Jackie Pettway, Stacy Howington, and Chris Kees.

The project has partially supported three students. Jill Reese received her degree in 2006 and is now employed at the Mathworks. Corey Winton should defend his thesis in early 2010 and formally graduate in May 2010. Winton is now employed at the Information Technology Laboratory at ERDC. Anna Meade is a new student and was supported by this project through May of 2010. she will be supported for the 2010–2011 academic year directly by ERDC though their BAA.

2 Results

We have published a paper [4] which compares several methods for optimal design of remediation strategies. This effort was supported by this project and the previous ARO funding.

Most of our efforts were directed at reduced order models for inverse problems in saturated flow. Such problems are a good first step to test ideas, enable us to integrate the optimization with ADH, and may lead to other applications, such as thermal inverse problems.

The computational cost of an ADH field-scale simulation in three dimensions is high, and it is important to reduce the number of expensive calls to the simulator. This is one of the reasons why the group at ERDC is not using methods like genetic algorithms or simulated annealing for calibration. Methods based on nonlinear least squares, however, miss the global features of the problem, and may converge to local minima that result in poor calibrations. One low cost approach to remedy this is to use a surrogate model or response surface to approximate the expensive objective function, minimize the surrogate with a global optimization method, and then sample the expensive function near one or more local minima of the surrogate.

We are using a POD (principal orthogonal decomposition) surrogate model [6, 8, 14, 16] which is a reduced order model used in the fluids control community. POD uses a basis which is built from several runs of the simulator, extracting a useful low-dimensional subspace with an eigenvalue calculation. We use a basis taken from the sensitivity vectors, which can be computed efficiently within finite element simulators like ADH. The student involved in this part of the project is Corey Winton, who is now employed at ERDC. Winton has been integrating the POD ideas directly into ADH, and we have attached a report by Winton (see § 2.1) on the details. The major advance in the last twelve months is the integration of a well model into the POD formulation. Winton should complete his Ph. D. work by the end of 2010. He has some significant, but manageable, computing left to do.

Our results to date are promising [12, 13] but we must have the results which use the well model before publishing in a journal. The well model is required because the problems of interest at ERDC have integrated flux boundary conditions, and the well model maps those boundary conditions into pressure boundary conditions. § 2.1 will explain the issues in detail.

Once the well model is in hand, we have publications (including Winton's thesis) prepared and waiting for it, as well as a collaboration with Farthing to create a hybrid method that uses the POD approximation with the genetic algorithm from [2] in the global phase, and with PEST [3] when the iteration is near convergence. While genetic algorithms are based on heuristics, there are methods to couple reduced order models and heuristic algorithms with rigorous optimization methods to obtain convergence results [1]. Hence, we expect the methods we design to have rigorous convergence properties.

2.1 Report by Corey Winton

In the past year, we have continued our application of Proper Orthogonal Decomposition (POD) on groundwater models. Our goal is to generate a reduced model using POD that will allow us to estimate the parameters that govern groundwater flow. The parameters we are most concerned with are hydraulic conductivity, the measure of velocity of a liquid through a porous medium.

This year, our progress has focused on the development and implementation of the total flux boundary condition. In previous years, we had solved

$$\nabla \cdot (K \nabla h) = f \text{ in } \Gamma \tag{1a}$$

$$\frac{\partial h}{\partial n} = 0 \text{ on } \partial\Gamma_1 \tag{1b}$$

$$h = g \text{ on } \partial\Gamma_2 \tag{1c}$$

We now seek to solve the following equation:

$$\nabla \cdot (K \nabla h) = f \text{ in } \Gamma, \tag{2}$$

but with the boundary condition

$$\Gamma = \Gamma_D \cup \Gamma_N \cup \Gamma_Q, \tag{3}$$

where

$$\Gamma_D = \quad \Gamma_{d_1} \cup ... \cup \Gamma_{d_{Nd}}, \tag{4a}$$

$$\Gamma_N = \quad \Gamma_{n_1} \cup ... \cup \Gamma_{n_{Nn}}, \tag{4b}$$

$$\Gamma_Q = \quad \Gamma_{q_1} \cup ... \cup \Gamma_{q_{Nq}}, \tag{4c}$$

and

$$\Gamma_{d_i} \Rightarrow \qquad h = \alpha_{d_i} \text{ on } \Gamma_{d_i}, \tag{5a}$$

$$\Gamma_{n_i} \Rightarrow \qquad \tfrac{\partial h}{\partial n} = \beta_{n_i} \text{ on } \Gamma_{n_i}, \tag{5b}$$

$$\Gamma_{q_i} \Rightarrow \quad \textstyle\int_{\Gamma_{q_i}} \tfrac{\partial h}{\partial n}\, dS = \phi_{q_i} \text{ on } \Gamma_{q_i}. \tag{5c}$$

The solution to (2) is given by

$$h = h_0 + \sum_{Nq} \gamma_i h_i, \tag{6}$$

where h_0 and h_i are solutions to (2) boundary conditions modified as follows:

- To solve for h_0, we leave Γ_D and Γ_N as defined in (4), (5), but force $h = 0$ on Γ_Q

- To compute h_i, we set $h = 0$ on Γ_D, $\dfrac{\partial h}{\partial n} = 0$ on Γ_N, and $h = 1$ on Γ_Q
- The N_q coefficients γ_i are derived from the following system of N_q equations:

$$\int_{\Gamma_{q_j}} \frac{\partial h_0}{\partial n}\, dS + \sum_{i=1}^{N_q} \gamma_i \int_{\Gamma_{q_j}} \frac{\partial h_{q_i}}{\partial n}\, dS = \phi_{q_j},\ j = 1...N_q. \tag{7}$$

For the reduced model, we compute the solutions h_i in (6) with

$$\left(A_0 + \sum_i^n A_i k_i\right) h_* = f_0^* + \sum_i^n f_i k_i. \tag{8}$$

That is, the only information that changes for each sub-solution h_i is contained in the vector f_0. The matrix A is constructed directly by our full model `ADH`. The vectors f are derived, but with minimal computational effort.

The total flux formulation with solution (6) serves several purposes:

- The total flux boundary on Γ_Q ensures a unique solution to (2)
- We have more information in our basis. Previously, the basis U was constructed with

  $$U = \left[h, \frac{\partial h}{\partial k_1}, \ldots, \frac{\partial h}{\partial k_n}\right],$$

  where k_i are the individual material conductivities found in K. Now, we have considerably more information and can build the basis

  $$U = \left[h_0, \frac{\partial h_0}{\partial k_1}, \ldots, \frac{\partial h_0}{\partial k_n}, h_1, \frac{\partial h_1}{\partial k_1}, \ldots, \frac{\partial h_1}{\partial k_n}, \ldots, h_{N_q}, \frac{\partial h_{N_q}}{\partial k_1}, \ldots, \frac{\partial h_{N_q}}{\partial k_n}\right].$$

  The expansion of the basis is significant as it this will allow the reduced order model to more accurately portray the physics of the full model.

- We are able to analytically compute the gradient for (6) with minimal additional effort. We see from (6) that

  $$\frac{\partial h}{\partial k_j} = \frac{\partial h_0}{\partial k_j} + \sum_{N_q} \left(\gamma_i \frac{\partial h_i}{\partial k_j} + \frac{\partial \gamma_i}{\partial k_j} h_i\right) \tag{9}$$

  We see from (8) that $\dfrac{\partial h_*}{\partial k_i}$ is given by

  $$A \frac{\partial h_*}{\partial k_i} = f_i - A_i h_*. \tag{10}$$

We can find $\frac{\partial \gamma_*}{\partial k_i}$ from (7)

$$\int_{\Gamma_{q_j}} \frac{\partial\left(\frac{\partial h_0}{\partial k_k}\right)}{\partial n}\, dS + \sum_{i=1}^{N_q}\left(\gamma_i \int_{\Gamma_{q_j}} \frac{\partial\left(\frac{\partial h_{q_i}}{\partial k_k}\right)}{\partial n}\, dS + \frac{\partial \gamma_i}{\partial k_k}\int_{\Gamma_{q_j}} \frac{\partial h_{q_i}}{\partial n}\, dS\right) = \phi_{q_j},\ j = 1...N_q \tag{11}$$

Each the terms in (11) are straightforward to solve. We construct a matrix M that allows us to compute the flux through any boundary Γ_j for a given solution h_i. That is,

$$Mh_i = \int_{\Gamma_j} \frac{\partial h_i}{\partial n}\, dS.$$

This matrix M does not change as we alter the boundary conditions, so it need only be constructed once.

It should be noted that the development and implementation of the total flux boundary condition is of interest not only in our optimization research, but also in the full `ADH` code. This boundary condition also serves as a useful well model for other applications. Rather than present the well as a prescribed flux through a set of elements, we can now solve for the accumulated flux through that boundary. The distinction is key – rather than assigning a flux at each element to simulate a well, we are now able to solve for the aggregate flux through that boundary.

Future Work We intend to use the reduced order model constructed by POD to pursue several optimization goals.

- First, we intend to show that an optimizer using POD will find at least a comparable local solution with less computational effort than if the optimizer used the full model in `ADH`.
- We aim to use POD with a Genetic Algorithm (GA) maintained by Matthew Farthing to find a global solution with less computational effort. A GA requires a large number of model simulations. We will demonstrate that the reduced model constructed by POD will allow the GA to investigate a large domain with significantly less computational effort than possible if it used the full model.

2.2 Other Research Efforts

We continue to collaborate with ERDC staff on multilevel solvers (Kees) grid optimization (Eslinger), and maintain discussions on temporal integration (Berger, Howington, Kees). We have recently published some theoretical studies on the method of pseudo-transient continuation [5,11,15,17], which we have helped put into ADH. We have also done theoretical work on nonlinear least squares [7, 10], which will have applications to our work on model calibration. The PI is also completing a book [9] on the implicit filtering algorithm, which we have been using for design of remediation systems [4].

3 Technology Transfer and Collaborations with ERDC

ERDC personnel use the work of the PI's group in many ways. Berger has used the work on pseudo-transient continuation in his surface water work. Our temporal integration code is now completely integrated into ADH, as is our work on preconditioning. We also work with Eslinger on optimization methods for mesh improvement.

Over the term of the project, Winton spent 8–12 weeks at ERDC in the summers of 2008 and 2009. Kelley visited ERDC at least twice each year of the project. Eslinger and Howington visited the PI at NC State University once each. The PI served on Hallberg's Ph. D. committee.

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